Light Element Opacities of Astrophysical Interest from ATOMIC

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We present new calculations of local-thermodynamic-equilibrium (LTE) light-element opacities from the LANL ATOMIC code [1] for systems of astrophysical interest. Our calculations, which include fine-structure detail, represent a systematic improvement over previous LANL opacity calculations using the LEDCOP legacy code [2]. The ATOMIC code uses ab initio atomic structure data computed from the CATS code, which is based on Cowan's atomic structure codes [3], and photoionization cross-section data computed from the LANL ionization code GIPPER [4,5]. ATOMIC also incorporates a new equation-of-state (EOS) model based on the chemical picture [6]. Our new calculations are made for elements of astrophysical interest and for a wide range of temperatures and densities.

Opacities are a crucial component in many areas of astrophysical modeling and are important to the programmatic mission of LANL. The opacities of the constituent elements of stars play an important role in the radiation transport through the stellar core and outer regions. Over the last 30 years, several worldwide groups have made great progress in generating the required opacities for elements of astrophysical interest. Collaborators within the Opacity Project (OP) have generated opacities for many elements [7,8,9]. The OPAL opacity database at LLNL [10] has provided mean opacity data for several sets of astrophysically relevant mixtures. The LANL OPLIB database has also provided opacity tables for wide ranges of temperatures and densities for many years, with the most recently available tables containing opacities generated using the LEDCOP code [2].

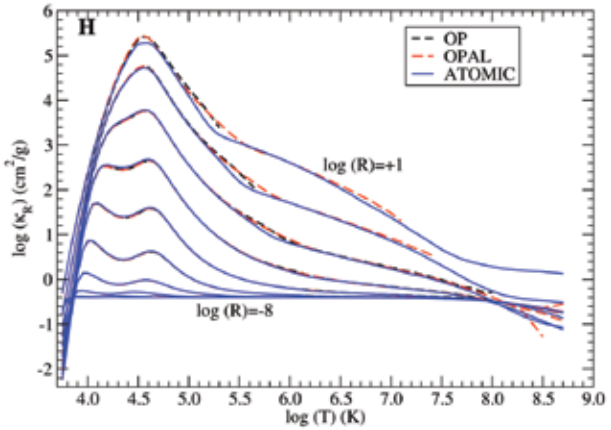

Fig. 1. Rosseland mean opacity of H as a function of log temperature (T) (in K). Each set of curves represents a constant log (R) value ranging from -8 to +1 as labeled. We compare the current ATOMIC calculations (solid blue curves) with OP calculations (short-dashed black curves) and OPAL calculations (dashed red curves).

Recently, we have completed new opacity tables for H through Ne using the ATOMIC code and are finalizing a new table for Fe. We aim to eventually supplant the opacity data in the OPLIB database that was generated from the legacy LEDCOP calculations, the last of which were made over 10 years ago, with data from our new ATOMIC calculations.

In Fig. 1 we compare our new hydrogen opacities with OP (short-dashed black lines) and OPAL (dashed red lines) calculations. The comparisons are made for a series of constant log (R) values, where $R=\rho/(T_6)^3$, and $T_6=10^{-6}T(K)$, for log (R) values from –8 to +1. We plot the logarithm of the Rosseland mean opacity as a function of log (T), with T the temperature (in Kelvin). Several features are evident from this comparison. Overall, excellent agreement is found between all the calculations, which encompass a wide range of temperatures and densities. The new ATOMIC results generally cover a wider range of temperatures than the OP and OPAL results.

There are several regions where differences between the methods may be found. At the highest temperatures of around 8.6 keV [corresponding to a log (T) of 8], there are some sizable differences between the ATOMIC and OPAL results. The OPAL data in this region are not particularly smooth as the temperature increases. In this fully ionized region, electron degeneracy effects and Pauli blocking are important, and the ATOMIC calculations incorporate these effects in a consistent manner. It is unclear how such non-ideality effects are included in the OPAL calculations.

At lower temperatures around 15–20 eV [log (T) around 5.2], we also observe some differences between the ATOMIC calculations and the OP and OPAL data (which also differ somewhat from each other). These differences are evident for only the highest density cases considered. The differences are due to small differences in the EOS model used, which causes the populations of excited states of the H atom to be different. In this region, the average ionization of the plasma is just under 1 (around 0.98), and most of the opacity arises from bound-free absorption from the weakly populated states of neutral H, which are very sensitive to the EOS model used. As the temperature increases, the plasma becomes fully ionized, and the three methods are again in excellent agreement.

In Fig. 2 we turn to a comparison of a monochromatic opacity, in this case for Fe. We plot the opacity for Fe for a single temperature (15.3 eV) and for a mass density of 5.5×10^{-3} g/cm^3. In this comparison we also present a LEDCOP calculation as shown by the red curve. We

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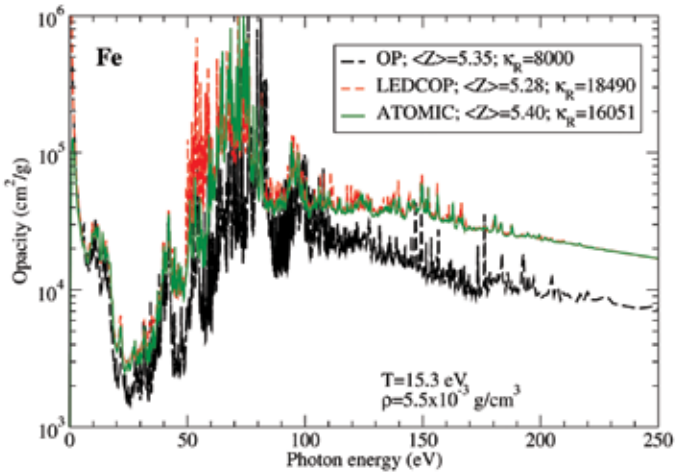

Fig. 2. Fe monochromatic opacity as a function of photon energy (in eV) for a temperature of 15.3 eV and a mass density of $5.5x10^{-3}$ g/cm^3. We compare the current ATOMIC calculations (solid green curve) with an OP calculation (dashed black curve) and a LEDCOP calculation (short-dashed red curve).

find that the OP monochromatic opacity is substantially lower (around a factor of two) than both the ATOMIC and LEDCOP calculations. The Rosseland weighting function peaks at around 60 eV and in this region the OP calculation is lower than the ATOMIC calculation by at least a factor of two. We also observe that at higher photon energies, where the opacity is dominated by bound-free contributions, the OP calculation is roughly a factor of two lower than both the ATOMIC and LEDCOP calculations. We note that these conditions are similar to those studied by other workers [11], where a variety of opacity calculations were presented. We find that the new ATOMIC calculations appear very similar to the hybrid calculations presented in [11], and similarly good agreement is found for the other temperatures and densities discussed in [11].

The ATOMIC and LEDCOP calculations presented in Fig. 2 are quite similar and produce a Rosseland mean opacity (κ_R) that agrees to within 15%. The primary reason for the 15% difference is the larger opacity observed in the LEDCOP calculation at around 55 eV. The opacity in this region is dominated by Δn=0 transitions within the 3p-3d transition array for several ion stages. Further investigations show that differences in the atomic structure calculations used in ATOMIC and in LEDCOP appear to be responsible for the larger LEDCOP opacity. The ATOMIC calculations include intermediate coupling within a configuration in the CATS structure calculations for a transition array. The LEDCOP calculation uses algebraic splitting of the configurations into terms, a procedure that does not account for intermediate coupling. This procedure produces oscillator strengths for the lower energy transitions within the 3p-3d transition array that are substantially larger than the oscillator strengths obtained from the intermediate coupling calculation, resulting in a larger overall opacity. We regard the ATOMIC calculations as more accurate since they are based on more accurate atomic structure calculations.

In this highlight we have discussed new LANL calculations of LTE opacities using the ATOMIC code. We have completed calculations for the elements H through Ne and the calculation of our new opacity table for Fe is well underway. We plan to perform more comprehensive calculations for all elements up to Zn in the next few years.

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